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HEADS UP!

Brian Patterson

Experiencing the finer aspects of materials in three dimension

By Diana Del Mauro
ADEPS Communications

If George Lucas visits Los Alamos, his first stop might be Brian Patterson's laboratory at the Target Fabrication Facility, where three-dimensional (3D) imaging happens on the nanoscale.

Patterson, a materials chemist, keeps a pair of 3D glasses handy so guests can experience the full effect of his movies. In a series of images impressive enough for the silver screen, a ladybug appears to leap from Patterson's computer screen and spin in all directions, exposing its circulatory system and muscles from the inside out.

Reviving the creature through micro x-ray computed tomography is a good exercise; however, Patterson's main mission is to magnify structures too small to be seen in materials, as well as the internal structures of high explosives, aerogels, carbon fiber composites, and foams. Patterson's movies illuminate a material's hidden flaws to a level of detail not previously available at the Laboratory.

"I like to tell people I have the best job on the Hill," he said. Rather than creating a separate image for each eye, as Hollywood does, Patterson's movies start with a series of single images. He reconstructs a two-dimensional image and computer software makes a 3D rendering of it. "The software gives one image to the left eye and the right eye simultaneously," he said.

Since 2006, Patterson has brought new ways of seeing to Polymers and Coatings (MST-7). "New instrument design and development, software development, and image manipulation—all in 3D—are at the forefront of my current research," he said.

Aiding his efforts are some powerful tools. Last year, the Laboratory purchased an Xradia UltraXRM-L200 microscope, the seventh of its kind in the country. Not only does it provide startling details about materials, it also gives researchers experience in 3D imaging on the nanoscale, preparing them for the sort of studies planned for the MaRIE (Matter-Radiation Interactions in Extremes) experimental facility.



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I am honored that Susan Seestrom selected me as Division Leader for MST. I'd also like to thank the selection committee for its hard work and time put into the process. This Division has a long history of materials leadership at Los Alamos—and internationally as well—and I look forward to working with all of you to continue leading materials science into the future. Although I know many of you, I welcome the opportunity to meet with all of the staff in MST Division. So, if you ever have an issue you would like to discuss, please come by. I have an open door policy, and although it may sometimes be hard to find me in my office, I will always make time to meet with you.

As we venture forward, I'd like to give a couple of thoughts on two near-term issues affecting the future of our Division: the Voluntary Separation Program and new science and manufacturing initiatives.

The Voluntary Separation Program (VSP) will be creating significant changes for many of us. For those employees considering leaving, this may be a difficult decision affecting both their careers and their lives. We will miss those that have decided it is their time to leave and will continue to value those that decide to continue serving the Laboratory. It is possible that the results of the VSP may cause us to have areas with weakened capability. Therefore, we may need to adjust staff assignments to balance our capabilities and to ensure that our critical capabilities are healthy moving forward. This may add to our already stressful environment amidst all of the other budgetary pressures. If you feel overstressed here are a few things that you can try to do to decrease your stress level: take a break, exercise or go for a walk, talk to your supervisor or colleagues, or see HR for stress management tools. Please watch out for your co-workers as well and try to help them through these stressful times.



'This Division has a long history of materials leadership at Los Alamos — and internationally as well — and I look forward to working with all of you to continue leading materials science into the future.'

Materials science at the national level is gaining attention from the highest levels in government. The President announced two new initiatives in June 2011: the Materials Genome Initiative and the Advanced Manufacturing Partnership. At the simplest level, these initiatives are aimed at developing new manufacturing processes and materials twice as fast using half as much energy and helping businesses operate at less cost. This past week I attended the TMS Manufacturing Summit, which brought together technical leaders from industry, academia and national laboratories to discuss how the community can respond to the challenges of the Advanced Manufacturing Partnership. Likewise, the Office of Basic Energy Sciences is launching a new initiative aimed at understanding materials behavior at the mesoscale and linking our atomistic understanding with the macro/continuum scale. This is an exciting time for materials science and I believe a great opportunity for MST Division to become a major leader in these national initiatives. Below are some links where you can learn more, and I welcome the opportunity to discuss any ideas you may have for engaging in these areas.

MST Division Leader David Teter

Materials Genome Initiative:

www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf

Advanced Manufacturing Partnership:

www.whitehouse.gov/the-press-office/2011/06/24/president-obama-launches-advanced-manufacturing-partnership

www1.eere.energy.gov/manufacturing/

BES Mesoscale Initiative:

meso2012.com/

Patterson... The new microscope offers the dual capabilities of ultra high-resolution x-ray radiography and 3D tomography with nanoscale resolution. "A human hair for this instrument is huge," Patterson said.

Patterson's first big thriller was when he exposed holes, as tiny as 200 nanometers in diameter, in a piece of copper that had been damaged in a gas gun experiment. "Not only can we visualize these features, but we can quantify their size and shape," he said.

The technology to achieve such an image, from any kind of device, is just a few years old. Previously, to get an image of this caliber, Los Alamos scientists travelled to a large synchrotron, such as Argonne National Laboratory's Advanced Photon Source. But now, within a few hours to a few days, Patterson can send a 3D-computed tomography image directly to their computer, saving time and money.

New to the studio

Though a fan of Jack Arnold's 1954 classic "Creature from the Black Lagoon," Patterson, who has a PhD in analytical chemistry, never dreamed he would become captivated by the finer points of 3D images. He was, he said, rather content as a high school science teacher at the time he entered graduate school.

In 2004, a whole new world opened up for Patterson, when George Havrilla (Chemical Diagnostics and Engineering, C-CDE) hired him as a postdoctoral researcher. Patterson began analyzing materials using x-ray fluorescence, something he knew nothing about, but easily grasped because of his spectroscopy experience at Ohio's Miami University. He also got his feet wet in 3D visualization techniques.

Havrilla said he now feels like a "proud papa" as Patterson makes a name for himself in a new field: x-ray tomography. "He's doing some really cool stuff with materials that go into weapons, on scales that no one has looked at before," Havrilla said.

As a result of ongoing collaborations between Patterson and Havrilla, Los Alamos weapons designers can see for the first time what causes corrupting high-density particles that could ruin test shots. They can change their processes and eliminate bad parts. The benefit: increased yield in well-characterized parts for testing.

That's just the kind of blockbuster that Los Alamos scientists have been waiting for.

Watch one of Patterson's movies at:
www.lanl.gov/orgs/mst/mst7/patterson.shtml.

Brian Patterson: My favorite experiment

What: Infrared imaging using a large germanium crystal

Why: So we could spectroscopically image the cross section of silicone foams.

When: 2006

Where: As a postdoctoral researcher in George Havrilla's lab (Chemical Diagnostics and Engineering, C-CDE)

Who: Havrilla and Patterson

How: I had an idea for a method to improve infrared microscopic imaging using a larger-than-typically-used germanium crystal. George and I wanted to detect the contamination due to residual catalyst within silicone foams. Scientists typically take a 3-millimeter diameter crystal, bring the sample into contact with the face, and raster the two through the infrared beam to collect an image. My idea was to use a much larger crystal, 25-millimeter in diameter, to lessen the optical aberrations and increase the imaging area.

The a-ha moment: After the calculations showed that it would work, we performed the experiment and we were able to collect an image area 100 times larger than previously demonstrated. We published it in *Applied Spectroscopy*. It was my favorite experiment in that I was able to take my original idea, do the calculations to show it would work, demonstrate the technique, and then publish it.

Wang to chair accelerator conference

Yongqiang Wang (Materials Science in Radiation and Dynamics Extremes, MST-8) will co-chair the 22nd International Conference on the Application of Accelerators in Research and Industry to be held Aug. 5-10 in Fort Worth, Texas.



Wang will help run this year's conference and prepare to serve as a future principal co-chairman of CAARI. He has been active in the conference since 1990, giving presentations, chairing sessions, and serving as topic editor for radiation effects.

Started in Oak Ridge in 1968, CAARI is a biennial international conference forum focusing on accelerator applications. Research topics to be covered at CAARI-2012, sponsored by the University of North Texas and Sandia National Laboratories, include accelerator technology; atomic physics; early-career research; ion beam analysis; ion beam modifications; medical applications; nanoscience and technology; nuclear-based analysis and energy; nuclear physics; radiation effects and production; safety, security and contraband detection; and teaching with accelerators.

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Wang... Since 2003, Wang has been team leader of the Ion Beam Materials Science Laboratory. Wang, who holds a PhD in nuclear physics and technology from Lanzhou University, China, is an author or co-author of more than 140 peer-reviewed publications, including three invited book chapters, and holds 1 U.S. patent. He co-edited the *Handbook of Modern Ion Beam Materials Analysis*, second edition, published in 2009 by the Materials Research Society through Cambridge University Press.

Technical contact: Y. Wang

LANL researchers invited to speak at UT Homeland Security Workshop

A team Los Alamos researchers presented invited talks at the recent Homeland Security Workshop at the University of Texas at Arlington.

The workshop was hosted by UTA physics professor Wei Chen, principle investigator for a DTRA- (Defense Threat Reduction Agency) funded project on scintillator development. The team of invited speakers from LANL discussed the relevant nuclear physics, detection strategies, optics and chemistry associated with scintillation and materials development. Ed McKigney (Transport Applications, XCP-7) spoke on nuclear physics as it relates to scintillation; Nickolaus Smith (MST-7) on synthetic methods of making scintillating materials; and Markus Hehlen (MST-7) on optical physics of rare earths.



Pictured clockwise from left, at the Homeland Security Workshop at UT Arlington, Marrius Hossu (UTA, visiting scientist), Markus Hehlen (MST-7), Andrew Brandt (UTA, physics professor), Rasool Kenarangui (UTA, nuclear engineering professor), Ryan Hall (UTA, graduate student in Wei Chen's group), Ed McKigney (XCP-7), Wei Chen (UTA, physics professor), Nickolaus Smith (MST-7), Kevin Lun (UTA, postdoctoral fellow in Wei Chen's group).

The afternoon sessions included a meeting with the provost, Dr. Ronald Elsenbaumer, a tour of Dr. Chen's laboratories and break out discussions with Prof. Chen's research group. The workshop provided the opportunity to help Dr. Chen's group with some research problems as well as to open the doors for future collaborative work between UTA and LANL.

Technical contact: N. Smith

Paper by MST researchers featured on front page of *Phys. Rev. B* Web site

Localized vibrational states in crystals are usually associated with extrinsic defects that break the translational invariance of the lattice. A different and evidently rare type of localized mode is associated with the vibration of "loose" atoms that occupy specific, oversized crystallographic sites. These so-called "rattling modes" were first identified about 50 years ago, but until recently few examples were known and they attracted little attention. During the past 15 years dozens of new materials that contain rattling modes have been discovered. In virtually all of these materials the rattling is accompanied by interesting physical phenomena, most notably a large reduction in lattice thermal conductivity, sizeable electron mass enhancements, and superconductivity. The reduced thermal conductivity has recently been exploited to develop new thermoelectric materials and devices with enhanced figures of merit. The heavy electron and superconducting behavior raise fundamental questions regarding electron-phonon and electron-electron coupling, and thus rattling modes are an active area of research in condensed matter physics.

To understand the role of rattling in these phenomena, one must first understand the details of the rattling vibration, particularly its anharmonicity. In their recent *Phys. Rev. B* paper "Localized anharmonic rattling of Al atoms in $\text{VA}_{10.1}$," Doug Safarik (Metallurgy, MST-6), Tomasz Klimczuk (formerly MST-8, now Institute for Transuranium Elements), Anna Llobet (Lujan Neutron Scattering Center, LANSCE-LC and MST-6), Darrin Byler (MST-8), Jason Lashley (MST-6), Jim O'Brien, and Neil Dilley (both Quantum Design Inc.) used diffraction, thermodynamic, and transport measurements to study the rattling of Al guest atoms in the intermetallic VA_{10} . They showed that each Al guest rattles in a square-well-like interatomic potential, so that the vibration is akin to a quantum-mechanical particle-in-a-box. The huge anharmonicity of this vibration facilitates its strong coupling to the acoustic phonons and conduction electrons, which in turn impedes heat and electrical transport. Their results suggest that the particular shape of the anharmonic potential

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HeadsUP!

Workplace uncertainty may lead to stress

Budget shortfalls are leading the Lab to take steps to address the monetary gap. Some employees are thinking about whether they want to take advantage of a Voluntary Separation Plan; others may be worrying about what other actions Lab management might take in the near future.

When people are faced with potential changes over which they have no control, they often respond with a wide range of emotions. Feeling worried or depressed also creates distractions, which increases the potential for accidents, injuries, and security violations. Learn what you can do to take better care of yourself. Please see lanl.gov/news/perspectives/2012/March/03.07_barber_perspectives.shtml.

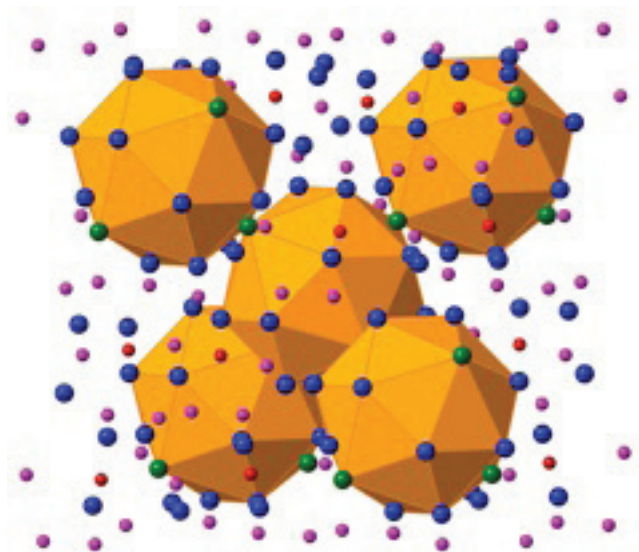
Need support? Call the Lab's Employee Assistance Program at 667-7339.

Adopt a parking lot; help prevent slips, falls

The new Adopt a Parking Lot program is a collaborative effort between the Industrial Hygiene and Safety (IHS) Division and WSSTs and organizations to enhance LANL's efforts to keep employees from getting hurt and parking lots safe. Nearly 60 slips, trips, and falls were reported at the Lab in December and January. The vast majority of these events occurred in parking lots.

Adopting a parking lot increases the focus on these areas and helps coordinate efforts to improve the conditions that lead to slips and falls. Read full article here: lanl.gov/news/news_stories/2012/February/02.14-adopt-a-parking-lot.shtml.

Want to help improve safety in a parking area? Call IHS Division Office at 606-0295 or email kristam@lanl.gov to indicate the parking area you're interested in adopting.



Featured on the *Phys. Rev. B* front Web page, a crystal structure of VAl_{10} emphasizing the diamond-like array of polyhedral cages, shown in orange. One Al guest atom rattles inside each cage.

Front... is important in determining the effect of rattling on the material's physical properties. By manipulating the chemistry and geometry of the rattling atom site, it may be possible to tune physical properties to create for example more efficient thermoelectric materials. Funding for the research was provided by Los Alamos's Laboratory Directed Research and Development program.

Technical Contact: *D.Safarik*

Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries this month:

Edward Orlor, MST-7	15 years
James Coy, MST-DO	10 years

MSTeNEWS

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To submit news items or for more information, contact Karen Kippen,
EPS Communications, at 606-1822, or kkippen@lanl.gov.

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To read past issues, please see www.lanl.gov/orgs/mst/mst_eneews.shtml.



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